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Estimate of 4-loop pole-$\overline{\text{MS}}$ mass relation from static QCD potential

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ABSTRACT

We estimate the presently unknown constant in the 4-loop relation between the quark pole mass and the $\overline{\text{MS}}$ mass, by requiring stability of the perturbative prediction for $E_{\text{tot}}(r) = 2m_{\text{pole}} + V_{\text{QCD}}(r)$ in the intermediate-distance region. The estimate is fairly sharp due to a severe cancellation between $2m_{\text{pole}}$ and $V_{\text{QCD}}(r)$. This would provide a test, based on general properties of the gauge theory, for the size of ultra-soft contributions to $V_{\text{QCD}}(r)$.

It has become an important theme of today's particle physics to precisely determine the masses of heavy quarks using the frame of perturbative QCD, as their values being indispensable inputs in various fields of modern particle physics. For the purpose of precisely determining heavy quark masses, often the relation between the pole mass and the mass in the modified-minimal-subtraction scheme ($\overline{\text{MS}}$ mass) of a quark becomes necessary. This relation can be expressed in a series expansion in the strong coupling constant as

$$m_{\text{pole}} = \overline{m}\left[1 + d_0\frac{\alpha_s(\overline{m})}{\pi} + d_1\left(\frac{\alpha_s(\overline{m})}{\pi}\right)^2 + d_2\left(\frac{\alpha_s(\overline{m})}{\pi}\right)^3 + d_3\left(\frac{\alpha_s(\overline{m})}{\pi}\right)^4 + \mathcal{O}(\alpha_s^5)\right]. \tag{1}$$

Here, $\overline{m} \equiv m_{\overline{\text{MS}}}(m_{\overline{\text{MS}}})$ denotes the $\overline{\text{MS}}$ mass renormalized at the $\overline{\text{MS}}$ mass scale; $\alpha_s(\mu) = \alpha_s^{(n_l)}(\mu)$ represents the strong coupling constant in the $\overline{\text{MS}}$ scheme, where n_l is the number of light quark flavors ($n_l = 3$, 4 and 5 for the charm, bottom and top quarks, respectively); the renormalization scale μ is set to $\overline{m}$. For the purpose of the analysis in this Letter, we use the coupling constant of the theory with n_l flavors only as the expansion parameter. The one-loop coefficient is given by $d_0 = 4/3$. The coefficients d_1 and d_2 are obtained from the two-loop [1] and three-loop [2][1] mass relations in the full theory (with n_h heavy quarks and n_l light quarks), respectively, by rewriting them in terms of the coupling constant of the theory with n_l light quarks only.[2] At present only limited part of d_3 are known [4,5], and there have been increasing demands for its full evaluation recently.

Major estimates of d_3 which have been performed so far rely on the renormalon dominance hypothesis of the pole mass [4,6–8]. (This includes the estimate in the so-called "large-β_0 approximation.") In these methods, there is an assumption (with certain grounds, see [9]) on the higher-order behavior of the perturbative expansion:

$$d_n \sim \text{const} \times n! n^{\beta_1/(2\beta_0^2)}\left(\frac{\beta_0}{2}\right)^n \quad \text{for } n \gg 1, \tag{2}$$

where β_i denotes the $(i+1)$-loop coefficient of the beta function of $\alpha_s(\mu)$. Empirically it is known that perturbative series of many observables are approximated well by this form even at relatively low orders. There have also been estimates of d_3 in another method [10].

In this Letter we present estimates of d_3 for $n_l = 0, 3, 4, 5$ based on comparatively general assumptions. In particular, our method does not use Eq. (2). We consider the total energy of a color-singlet pair of heavy quarks Q and $\bar{Q}$, defined by

$$E_{\text{tot}}(r) = 2m_{\text{pole}} + V_{\text{QCD}}(r). \tag{3}$$

The static QCD potential $V_{\text{QCD}}(r)$ represents the potential energy between Q and $\bar{Q}$ at a distance r, in the static limit. We require stability of the perturbative prediction of $E_{\text{tot}}(r)$ at relatively large r, within the range where the perturbative prediction is expected to be valid. Although originally this stability was predicted using the language of the renormalon dominance hypothesis [11], it can be considered to hold as a general property of perturbative QCD beyond the renormalon dominance hypothesis [12]. In fact, a gluon, which couples to static currents $j_a^\mu \propto \delta^{\mu 0}$, couples to the total charge of the system $Q_a^{\text{tot}} = \sum_i j_{a,i}^0(q=0)$ $(i = Q, \bar{Q})$ in the zero momentum limit $q \to 0$, that is, an infra-red (IR) gluon decouples from the color-singlet system. Diagrammatically an IR gluon

[1] The same relation was obtained before in [3] in a certain approximation.

[2] This relation coincides with Eq. (14) of [2]. Note that in the other formulas of [2], the coupling constant of the full theory is used.

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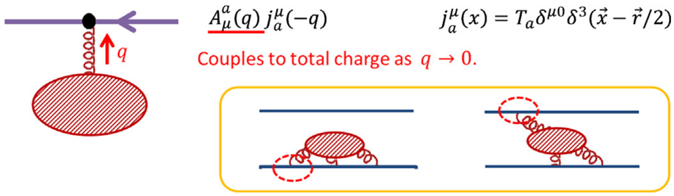

Fig. 1. As a general feature of the gauge theory, a gluon, which couples to static currents $j^\mu_a \propto \delta^{\mu 0}$, couples to the total charge of the system in the IR limit, $q \to 0$. Diagrammatically both self-energy and potential-energy type diagrams are needed for realizing this feature, hence, for a color-singlet system, a cancellation takes place between the two types of diagrams.

observes the total charge when both self-energy diagrams[3] and potential-energy diagrams are taken into account. Hence, a cancellation takes place between these two types of diagrams, see Fig. 1. In perturbative QCD, convergence and stability of perturbative series become worse as contributions from IR gluons grow. Oppositely, after cancellation of IR contributions, convergence and stability of perturbative predictions improve. This can be considered as a general property of a gauge theory which is strongly interacting at IR.

In the perturbative series of $E_{\text{tot}}(r)$ up to $\mathcal{O}(\alpha_s^3)$, where the exact terms are known, an improvement of convergence and stability as a result of the cancellation is clearly visible, and the cancellation becomes severer at higher orders. The meaning of the latter statement is as follows. The perturbative series of m_{pole} and $V_{\text{QCD}}(r)$, respectively, do not converge well, whereas the perturbative series of $E_{\text{tot}}(r)$ converges much more quickly. Let us denote the individual terms of the former as m_n and V_n, respectively, and of the latter as E_n. Then the ratio $|E_n/m_n|$ or $|E_n/V_n|$ reduces with n. This means that there is a severer cancellation for larger n: $(2|m_n| - |V_n|)/(2|m_n| + |V_n|) \approx E_n/(2|V_n|)$. As a consequence, by assuming convergence and stability of $E_{\text{tot}}(r)$ up to the next order [$\mathcal{O}(\alpha_s^4)$], we obtain fairly severe constraints on our estimates of d_3.

The leading IR contributions being canceled in the static limit, let us consider the next-to-leading IR contributions which may affect the stability of the perturbative prediction for $E_{\text{tot}}(r)$. The interaction of the singlet static $Q\bar{Q}$ pair and IR gluons starts from a dipole interaction $S\,\vec{r}\cdot\vec{E}^a\, O^a$ in the multipole expansion in $\vec{r}$ [13]. The ultra-soft (US) corrections to $V_{\text{QCD}}(r)$ originating from this interaction appear first at $\mathcal{O}(\alpha_s^4)$. It has been argued that the US corrections are small at this order [14]. There also exist arguments that these corrections may not be small [7]. In our analysis, we assume that these corrections are small and estimate d_3 by requiring stability of the perturbative prediction for $E_{\text{tot}}(r)$ in an IR region.[4] Subleading IR contributions to m_{pole}, which may also affect the stability of $E_{\text{tot}}(r)$, are expected to be suppressed by $\Lambda_{\text{QCD}}/\overline{m}$. By increasing $\overline{m}$, we render these contributions sufficiently small.

Let us review the behavior of the perturbative series of $E_{\text{tot}}(r)$ up to $\mathcal{O}(\alpha_s^3)$ at relatively large r, as analyzed in [15]. Comparing the perturbative series in $\alpha_s(\mu)$ of $E_{\text{tot}}(r)$ and those of m_{pole} and $V_{\text{QCD}}(r)$ individually, we observe a drastic improvement in convergence of the series. In the case $n_l = 4$, $\overline{m} = 4.180$ GeV and $\alpha_s(M_Z) = 0.1184$, a stable theoretical prediction for $E_{\text{tot}}(r)$ is obtained at $r < 2.8\ \text{GeV}^{-1}$. At each r, the scale μ is fixed in two different ways: (1) The scale $\mu = \mu_1(r)$ is fixed by demanding stability of $E_{\text{tot}}(r)$ against variation of the scale (minimal-sensitivity scale [16]):

$$\mu \frac{d}{d\mu} E_{\text{tot}}(r)\,\Big|_{\mu=\mu_1(r)} = 0. \tag{4}$$

(2) The scale $\mu = \mu_2(r)$ is fixed on the minimum of the absolute value of the $O(\alpha_s^3)$ term E_3 of $E_{\text{tot}}(r)$:

$$\mu \frac{d}{d\mu} (E_3)^2\,\Big|_{\mu=\mu_2(r)} = 0. \tag{5}$$

Here and hereafter, we state that a stable theoretical prediction is obtained when both scales exist; in this case, we find that the values of $E_{\text{tot}}(r)$ corresponding to both scales agree well, and that the convergence behaviors of both expansions are reasonable. The range of stable prediction extends to larger r as the order of perturbative expansion is raised [up to $\mathcal{O}(\alpha_s^3)$].

$E_{\text{tot}}(r)$ is examined also by varying the value of $\overline{m}$ artificially: whenever stable theoretical predictions for $E_{\text{tot}}(r)$ are obtained, the predictions corresponding to different $\overline{m}$ agree with each other within the estimated theoretical uncertainties, after adding an arbitrary r-independent constant. [Theoretical uncertainties are estimated as order $\Lambda_{\text{QCD}}^3 r^2$ with $\Lambda_{\text{QCD}} \simeq 300$ MeV.] As $\overline{m}$ is increased, the perturbative predictability range of r, where both scales exist, shifts to shorter-distance region. These examinations may be regarded as tests of properties of the $SU(3)$ gauge theory, irrespective of details of the parameters of the theory.[5]

Phenomenologically $E_{\text{tot}}(r)$ is compared with typical phenomenological potentials. They are in agreement in the relevant distance range, $0.5\ \text{GeV}^{-1} \lesssim r \lesssim 2.8\ \text{GeV}^{-1}$, within the estimated theoretical uncertainties, after adding an arbitrary r-independent constant to each potential; this is the case independently of the value of $\overline{m}$ (as long as a stable prediction is obtained), but only in the cases where realistic values are chosen for $\Lambda_{\overline{\text{MS}}}$.[6] There are also similar comparisons with lattice computations of $V_{\text{QCD}}(r)$, with good agreements [19,20].

Now we repeat the same analysis including the terms at the next order and varying d_3 in addition. We first set $\alpha_s(M_Z) = 0.1184$, $\overline{m} = 4.180$ GeV and $n_l = 4$. (We neglect the masses of the light quarks in the following analysis.) We take for $V_{\text{QCD}}(r)$ the sum of the perturbative series up to $\mathcal{O}(\alpha_s^4)$ [21,22] and $\mathcal{O}(\alpha_s^4 \log\alpha_s)$ [13,23], as given by Eq. (21) of [24]; the $\mathcal{O}(\alpha_s^4 \log\alpha_s)$ term is generated by contributions from the US scale. Roughly speaking, if we choose a value of d_3 close to that of the renormalon estimate [6] or to the large-β_0 value [4]

$$d_3(\text{large-}\beta_0) \simeq 3046.29 - 553.872 n_l + 33.568 n_l^2 - 0.678141 n_l^3, \tag{6}$$

a cancellation between $2m_{\text{pole}}$ and $V_{\text{QCD}}(r)$ takes place and a relatively convergent and stable prediction is obtained. Nevertheless, the level of cancellation depends sensitively on the value of d_3. For demonstration we show in Fig. 2 the scale dependences of $E_{\text{tot}}(r)$ at $r = 2.8\ \text{GeV}^{-1}$, and $d_3 = 0.95 \times d_3(\text{large-}\beta_0)$. Four solid lines are

[3] In the large mass limit contributions from IR region to the pole mass approximate IR contributions to the self-energy of a static charge.

[4] In terms of the renormalon language, our standpoint may be phrased as follows. Since there exist uncanceled IR renormalons in $E_{\text{tot}}(r)$, starting from the $u = 3/2$ pole in the Borel plane, they may deteriorate convergence of the perturbative series at higher orders of the perturbative expansion. Ultra-violet (UV) renormalons may also contribute. We assume that both of these contributions are small and negligible in estimating d_3.

[5] In this analysis, the parameters of the theory can be taken as a dimensionful parameter $\Lambda_{\overline{\text{MS}}}$ (which sets the unit of mass dimension) and a dimensionless parameter $\overline{m}/\Lambda_{\overline{\text{MS}}}$. Hence, we may vary only $\overline{m}$ fixing $\Lambda_{\overline{\text{MS}}}$, so that we can always consider Λ_{QCD} to be of the order of 300 MeV.

[6] These features may be summarized as follows. Whenever a stable prediction is obtained, $E_{\text{tot}}(r)$ is consistent with a function of the form $\Lambda_{\overline{\text{MS}}} \times f(\Lambda_{\overline{\text{MS}}} r)$ up to an additive constant, where $f(x)$ is independent of $\overline{m}$; only when a realistic value of $\Lambda_{\overline{\text{MS}}}$ is chosen it is consistent with phenomenological potentials. In fact, such a function $f(\Lambda_{\overline{\text{MS}}} r)$ can be explicitly extracted from $V_{\text{QCD}}(r)$ as a short-distance dominant (renormalon-free) part, given as a "Coulomb+linear" potential [17,18].

Table 1
Comparison of different estimates of d_3 defined in Eq. (1). The estimate of Ref. [4] denotes $d_3(\text{large-}\beta_0)$; those of Refs. [6,7] and [8] are based on the renormalon hypothesis; the estimate of Ref. [10] is derived by an effective charge method.

n_l	Ref. [4]	Ref. [6]	Ref. [7]	Ref. [10]	Ref. [8]	Our estimate
0	3046.29	3706.78	–	–	3933.01	$(1.1 \pm 0.05) \times d_3(\text{large-}\beta_0) \approx 3351^{+152}_{-152}$
3	1668.48	1818.60	1785.9	1281	–	$(1.0 \pm 0.1) \times d_3(\text{large-}\beta_0) \approx 1668^{+167}_{-167}$
4	1324.49	1345.72	1316.4	986	–	$(0.95^{+0.02}_{-0.05}) \times d_3(\text{large-}\beta_0) \approx 1258^{+26}_{-66}$
5	1031.37	947.90	920.1	719	–	$(0.87^{+0.03}_{-0.17}) \times d_3(\text{large-}\beta_0) \approx 897^{+31}_{-175}$

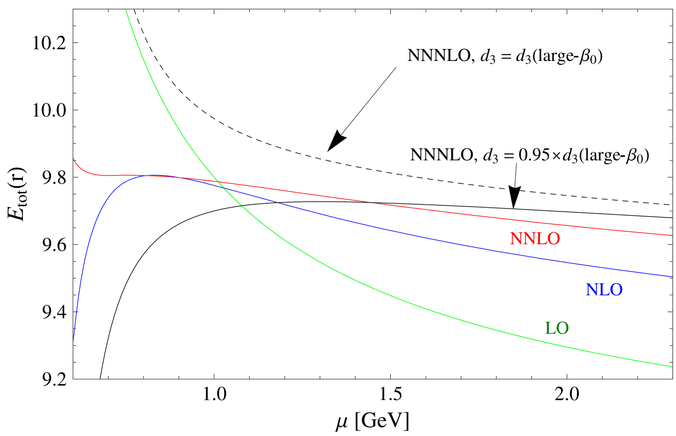

Fig. 2. $E_{\rm tot}(r)$ at $r = 2.8\ \text{GeV}^{-1}$ as a function of the scale μ. The solid lines represent the sum of the perturbative series up to $\mathcal{O}(\alpha_s)$ [LO], $\mathcal{O}(\alpha_s^2)$ [NLO], $\mathcal{O}(\alpha_s^3)$ [NNLO] and $\mathcal{O}(\alpha_s^4)$ [NNNLO, $d_3 = 0.95 \times d_3(\text{large-}\beta_0)$]. The dashed line represents the NNNLO prediction corresponding to $d_3 = d_3(\text{large-}\beta_0)$. We set $\alpha_s(M_Z) = 0.1184$, $\overline{m} = 4.180$ GeV and $n_l = 4$.

plotted, corresponding to the sum of the perturbative series up to $\mathcal{O}(\alpha_s)$ [LO], $\mathcal{O}(\alpha_s^2)$ [NLO], $\mathcal{O}(\alpha_s^3)$ [NNLO] and $\mathcal{O}(\alpha_s^4)$ [NNNLO]. The next-to-next-to-next-to-leading order (NNNLO) prediction corresponding to $d_3 = d_3(\text{large-}\beta_0)$ is also shown with a dashed line.

As already stated, at NNLO both scales $\mu_1(r)$ and $\mu_2(r)$ [Eqs. (4) and (5)] exist up to $r \simeq 2.8\ \text{GeV}^{-1}$. We require that at NNNLO both scales also exist at least up to the same r, such that the perturbative stability is not deteriorated at this order. This requirement leads to an upper bound for d_3: $d_3 < 0.96 \times d_3(\text{large-}\beta_0)$. We also vary $\overline{m}$ artificially to 8 GeV and 16 GeV and require that at NNNLO the two scales exist at least up to the same r as at NNLO. (The corresponding values of r are 1.4 GeV^{-1} and 0.7 GeV^{-1}, respectively.) In these cases, a common value $0.97 \times d_3(\text{large-}\beta_0)$ is obtained as upper bounds for d_3. All the upper bounds are fairly solid, in the sense that as soon as we assign a larger value to d_3 in each case, we observe a strong instability of the perturbative prediction; see Fig. 2. Since all the upper bounds are of similar values, we consider that effects of $1/\overline{m}$-suppressed contributions to $m_{\rm pole}$ are sufficiently small and take $0.97 \times d_3(\text{large-}\beta_0)$ as the reference value for the upper bound of d_3 of our estimate.

If we assign a value much smaller than $d_3(\text{large-}\beta_0)$ to d_3, qualitatively the perturbative series of $E_{\rm tot}(r)$ at NNNLO tends to become unstable and exhibit a poorer convergence behavior. For instance, the scales fixed at NNLO and NNNLO [Eq. (4) or Eq. (5)] tend to be separated farther; the crossing points of the solid lines in Fig. 2, which are centered to a small region, tend to be separated apart. We quantify this feature by further demanding that the difference between the NNLO and NNNLO predictions be smaller than the perturbative uncertainty[7] $\Lambda_{\rm QCD}^3 r^2$ ($\Lambda_{\rm QCD} = 300$ MeV) for each of the scale choices $\mu = \mu_1(r)$ and $\mu = \mu_2(r)$; since the estimate $\Lambda_{\rm QCD}^3 r^2$ is meaningful only in an IR region, we apply this requirement in the range $r > 1\ \text{GeV}^{-1}$. This requirement sets a lower bound for d_3 corresponding to each value of $\overline{m}$.[8] We obtain $d_3 \gtrsim 0.90 \times d_3(\text{large-}\beta_0)$. This value, however, depends on our choice $\Lambda_{\rm QCD} = 300$ MeV. Thus, in comparison to the upper bound, the lower bound is to some extent obscure.

After choosing a value of d_3 within the range determined by the above two requirements, qualitatively the perturbative prediction for $E_{\rm tot}(r)$ becomes stable and the perturbative series exhibits an optimally convergent behavior. This effect is enhanced especially at larger r. An optimal estimate is $d_3 \approx 0.95 \times d_3(\text{large-}\beta_0)$; see Fig. 2. We repeat the same analyses for $n_l = 0$, 3 and 5 and find qualitatively similar results. Our estimates of d_3 are summarized in Table 1. Other estimates of d_3 are also listed in the same table for comparison. We note that the large-β_0 values and some of the renormalon estimates for $n_l = 4, 5$ lie above the upper bounds of our estimates.

Once d_3 is computed exactly in the future, a comparison with our estimates will test our understanding of the perturbative series of $E_{\rm tot}(r)$. In particular, it will test our assumption that the US contributions (the leading residual IR contributions in the multipole expansion that may affect the stability of the perturbative series) are small and do not deteriorate the perturbative convergence observed up to NNLO. Other assumptions are based on general properties of a gauge theory strongly interacting at IR and are independent of the renormalon dominance Eq. (2). We obtained fairly constrained estimates for d_3 reflecting a severe cancellation between $2m_{\rm pole}$ and $V_{\rm QCD}(r)$.

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[7] The estimate of order $\Lambda_{\rm QCD}^3 r^2$ is among the predictions of the renormalon dominance hypothesis. It can, however, be derived also in a more general framework, without assuming the renormalon dominance, Eq. (2). Namely, within the effective field theory "potential non-relativistic QCD" (pNRQCD), the leading IR contribution to $E_{\rm tot}(r)$ can be absorbed into a matrix element of a non-local gluon condensate, whose size is of order $\Lambda_{\rm QCD}^3 r^2$ by dimensional analysis [13]. In this case only UV contributions remain in the perturbative expansion of the Wilson coefficient, which should be more convergent than the perturbative series of $E_{\rm tot}(r)$. Thus, IR contributions to $E_{\rm tot}(r)$ generates (at most) order $\Lambda_{\rm QCD}^3 r^2$ uncertainties. (See also [18].)

[8] Since we require consistency with the NNLO prediction, the perturbative prediction of $E_{\rm tot}(r)$ at NNLO also agrees with typical phenomenological potentials if we take a realistic value for $\Lambda_{\overline{\rm MS}}$.

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